COUPLED-CLUSTER CALCULATIONS FOR LOW-LYING ELECTRONIC STATES OF HEAVY-METAL CONTAINING MOLECULES

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Coupled-cluster calculations of low-lying electronic states for heavy-metal containing diatomic molecules (e.g., PtH, ThO^+, ThN, BaO^+, CsF^+) are reported. Recently-developed relativistic quantum-chemical techniques have been used, including an atomic mean-field approach for efficent construction of spin-orbit integrals [1], a perturbative approach for treating spin-orbit coupling within exact-two-component equation-of-motion coupled-cluster methods [2], and a new implementation of two-component coupled-cluster methods for non-perturbative treatments of spin-orbit coupling [3]. Bond lengths, vibrational frequencies, and dipole moments of these molecules containing heavy metals are compared with experimental data to assess the accuracy and usefulness of the computational methods.

References

[1] J. Liu and L. Cheng, J. Chem. Phys. submitted.

[2] L. Cheng, F. Wang, J. F. Stanton, and J. Gauss, J. Chem. Phys. **148**, 044108 (2018).

[3] J. Liu, Y. Shen, A. Asthana, and L. Cheng, J. Chem. Phys. **148**, 034106 (2018).